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One-electron model of the high-frequency dielectric function of dense plasmas

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Abstract. The approach is developed to calculate reflectivity and high-frequency dielectric permeability of dense plasmas. The Kubo–Greenwood formula is applied. One-electron wave functions are used. Plane waves are substituted for the wave functions of the free states. Hydrogen-like wave functions are substituted for the wave functions of the bound states. The restriction of the excited pair bound states is included in the approach. Calculations are performed for the shock-compressed xenon. The results are in the fair agreement with the experimental data for densities $\rho > 2 \text{ g/cm}^3$ whereas the remarkable discrepancy appears at low densities. The discrepancy can be attributed to a finite width of the shock front. The width increases with the decrease of density and can contribute to the reflectivity at low densities.

1. Introduction
Measurements and theoretical analysis of reflectivity are conventional methods of phase diagram investigation [1,2], particularly in shock wave experiments where the number of the parameters measured is restricted. The refection of the shock-compressed xenon is measured in the unique experiments of Mintsev, Zaporozhets et al [3, 4]. The results turn out to be challenging for theorists and shows the necessity of a correct theory construction, which would give the description of the interaction of radiation with nonideal plasmas.

The quantum-mechanical approach with the linear response theory and the Kubo–Greenwood formalism [3] (section 1) are used for calculation of reflectivity in this paper. One-electron wave functions are applied for the calculations; classical molecular dynamics results are used to restrict the excited atomic states (section 2). The approach is applied to xenon plasma (section 3) studied in [4, 5]. The shock front broadening influence on the reflectivity is discussed at the low plasma densities.

2. Kubo–Greenwood method
The method gives the expression for the electric conductivity in the first order of the perturbation theory. The dependence on frequency $\omega$ of the real part of the conductivity $\sigma^{(1)}$ is defined by the following expression

$$\sigma^{(1)}(\omega) = \frac{\pi e^2 \hbar^2}{m^2 \omega \Omega} \sum_{n,n',k} 2[f(E_{n'k}) - f(E_{nk})] \left| \langle \psi_{n'k} | \nabla | \psi_{nk} \rangle \right|^2 \delta(E_{n'k} - E_{nk} - h\omega),$$  \hspace{1cm} (1)
where $e$ and $m$ are electron charge and mass, $\hbar$ is the Plank constant, $\Omega$ is a system volume, $k$ is a wave number of the incident radiation. The summation is carried out over all electron states $n$, $n'$. The contribution of the sum terms with $n = n'$ (intraband transitions) are taken into account as well as the contribution of the terms with $n \neq n'$ (interband transitions). The factor 2 allows for the electron spin-degeneracy. $f(T,E_{n,k})$ is the Fermi–Dirac distribution function at temperature $T$, which defines an occupation of a state $n$. $E_{n,k}$ is an eigenvalue (an energy level) corresponding to the wave function $\psi_{n,k}$. $\sigma^{(1)}$ is related to the imaginary part $\varepsilon^{(2)}$ of the dielectric function

$$\varepsilon^{(2)} = 4\pi \omega^{-1} \sigma^{(1)}. \quad (2)$$

The real $\varepsilon^{(1)}$ and imaginary parts of the dielectric function are connected by the Kramers–Kronig transformation

$$\varepsilon^{(1)}(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\varepsilon^{(2)}(\omega') \omega'}{\omega'^2 - \omega^2} d\omega', \quad (3)$$

where $P$ denotes the principle value (in the limit $\eta \to 0$).

3. One-electron model

One-electron approach is applied within the framework of the Hartree approximation. The system wave function of all the electrons in (1) is represented in the form of the product of one-electron wave functions. The approximation gives a satisfactory description of the non-degenerate plasma, when the exchange terms of the more accurate asymmetric product of the one-electron wave functions are not essential.

One-electron wave functions can be obtained from the solution the Schrödinger equation in the effective average field of the all other electrons of the system. Note that the average field can be obtained for the nondegenerate electron-ion plasma in the quasiclassical approximation, classical molecular dynamics included.

Plane waves can be used for the free electrons wave functions as the initial approximation

$$\psi_k = \Omega^{-1/2} \exp(ikr). \quad (4)$$

Hydrogen-like wave functions are substituted for the wave functions of the bound states. Effective principle quantum numbers $n_{\text{eff}}$ are used in the radial part of the wave functions to take into account the difference of the atom from the hydrogen atom. The energies are $E_n = -Z^2 R_y/n_{\text{eff}}^2$.

Coulomb microfields destroy the higher excited levels in plasmas. Therefore a restriction $|E_n| < E_{\text{gap}}$ of the excited pair bound states is included in the calculations. The boundary energy is found from the molecular dynamics simulations earlier [6, 7] as

$$E_{\text{gap}} = 2(4\pi/3)^{1/3} e^2 n_e^{1/3} [Z/Z_{\text{av}}^{1/3}]. \quad (5)$$

The average charge is $Z_{\text{av}} = \sum_k \alpha_k Z_k$, where $\alpha_k$ is a portion of ions with the charge $Z_k$.

An example of the densities of states of the xenon atom and ions is presented in figure 1 for a plasma density which is a typical one for the experimental conditions [4, 5]. Atomic and ionic energy levels are combined with the restriction (5) and results for the densities of states obtained by both the classical molecular dynamics simulation and quantum VASP density functional theory (DFT) computations.
4. Reflectivity

Results are presented in figure 2 for the reflectivity coefficients calculated for the wavelengths $\lambda = 694$ and $\lambda = 532$ nm. The expression (1) is applied within the framework of the above given approximations. The model developed yields satisfactory agreement with the experimental data at the high plasma densities. The discrepancy takes place at the low plasma density. The same discrepancy is the case for the DFT calculations [8].

The discrepancy can be attributed to the shock wave front broadening due to the finite rate of the ionization processes after the shock front. The inhomogeneous profile of the electron concentration in this layer influences the reflectivity character. The Fresnel formula is not valid anymore, which is used in [8]. The direct consideration is needed of the electrodynamics problem of the interaction of the incident radiation with the layer with the changeable dielectric function.

The authors [9–12] attempt to explain experimental results within the framework of the Drude model with an artificial broadening of the wavefront. It is assumed that the density in the shock-compressed xenon increases not abruptly but there is a transient region of finite width, in which the density increases smoothly to a final value. Thus, the wavefront has a finite width and the laser light is reflected not directly from the xenon plasma, but from the extended front. The assumption, that the wavefront width is about 1 $\mu$m, improves significantly the agreement with the experiment in comparison with the assumption of a sharp front, when the Drude formula is used. However, the effect of the front broadening has no independent experimental confirmation of the essential wavefront width needed.

The failure of [9–12] can be related to the inadequate reflectance which is used. Therefore, we applied our reflectance (figure 2) to treat the problem.

Consider a radiation which falls upon a plasma layer with an inhomogeneous dielectric function $\varepsilon_\omega(x)$. The electric field can be represented as $E_\omega(x,t) = E_0(x,t) \exp(i\omega t)$. It follows
Figure 2. Reflectivity dependence on the plasma density for \(\lambda = 694\) nm (A) and 532 nm (B): 1 is experiment [4, 5], 2 is DFT calculation [13], 3 is the result (1) for the one-electron model.

Table 1. Thicknesses of the inhomogeneous shock-front plasma layer estimated from the experimental reflectance data [4, 5].

<table>
<thead>
<tr>
<th>Plasma density, g/cm(^3)</th>
<th>0.51</th>
<th>1.1</th>
<th>1.6</th>
<th>2.2</th>
<th>2.8</th>
<th>3.4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Layer thickness(^+), nm</td>
<td>(\lambda = 532) nm</td>
<td>220</td>
<td>174</td>
<td>113</td>
<td>68</td>
<td>—</td>
</tr>
<tr>
<td></td>
<td>(\lambda = 694) nm</td>
<td>191</td>
<td>124</td>
<td>93</td>
<td>69</td>
<td>0</td>
</tr>
</tbody>
</table>

\(^+\)There are no experimental data [4, 5] for 0.51 and 3.4 g/cm\(^3\) at \(\lambda = 532\) nm.

from the Maxwell equations in this case that

\[
\omega^2 \varepsilon_\omega(x) E_0 c^{-2} + \nabla \left[ \frac{1}{\varepsilon_\omega(x)} (E_0 \nabla \varepsilon_\omega(x)) \right] = 0, \tag{6}
\]

where \(c\) is the light speed.

The dielectric function gradient is orthogonal to the electric field vector if the incident radiation is perpendicular to the plasma layer. Only one electric field vector projection is non-zero in this case. Therefore, the vector \(E_0\) can be substituted by its module \(E_0\). The equation (6) can be simplified to

\[
\omega^2 \varepsilon_\omega(x) E_0 c^{-2} + \Delta E_0 = 0. \tag{7}
\]

Suppose that the dielectric function depends on the coordinate \(x\) only for \(0 < x < x_0\): \(\varepsilon_\omega(x) = 1\) at \(x < 0\), and \(\varepsilon_\omega(x) = \varepsilon_\infty\) at \(x > x_0\), where \(\varepsilon_\infty\) is a dielectric permeability of the equilibrium plasma with the thermodynamic parameters behind the shock front. It allows formulating the boundary conditions as

\[
E_0(0) = 1 + r; \quad E_0(x_0) = d; \quad E'_0(0) = ik - ikr; \quad E'_0(x_0) = ik\varepsilon_\omega(x)^{1/2}. \tag{8}
\]

Here \(r\) and \(d\) are complex reflection and transmission coefficients for the inhomogeneous plasma layer, \(k\) is a wave number in vacuum. The simplest assumption is the linear dependence of \(\varepsilon_\omega(x)\) from 1 at \(x = 0\) till \(\varepsilon_\infty\) at \(x = x_0\).

A numerical solution of the problem (7) is obtained with the boundary conditions (8). It permits to estimate the thickness of the plasma layer, which matches the experimental data with the values of the dielectric function calculated (table 1). Discrepancies between layer thicknesses
obtained for 532 and 694 nm for the one and the same plasma density can be attributed to the more complex profile of the dielectric function than linear which is used in the calculations.

Note that the values of the layer thickness in the table 1 turn out to be close to the values about 160 nm obtained from the analysis of the Brewster angle for the same plasmas [14].

5. Conclusions
A model is developed which permits to estimate the high-frequency dielectric permeability of dense plasmas from the Kubo–Greenwood formula. One-electron wave functions and a restriction of the atomic levels due to the Coulomb microfields are used.

The results calculated agree with the experimental data at the high plasma densities. The discrepancy at the low plasma density is matched with the existence of the inhomogeneous plasma layer at the shock wave front.

The approximations used above for the wave functions are rather rough. The number of excited states, which are necessary to include into calculations, increases with the decrease of density. It is another source of an error to be removed at low densities.

Acknowledgments
The authors thank V B Mintsev and Yu B Zaporozhets for the information about the results of the measurements. The work is supported by the grant No. 14-19-01295 of the Russian Science Foundation.

References